Relativistic Effect on the Ionization Probability in the Geometrical Model

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Relativistic Effect on the Ionization Probability in the Geometrical Model

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Ionization probabilities in ion-atom collisions at zero impact parameter have been calculated with the relativistic hydrogenic wave functions in the geometrical model. The obtained results are shown graphically and compared with the nonrelativistic values. It is found that the relativistic effect increases the ionization probability significantly for s and $p_{1/2}$ electrons in heavy elements.

KEY WORDS: /Ionization probability/Geometrical model/Relativistic effect/

1. INTRODUCTION

In ion-atom collisions, the multiple ionization process has received a special attention both experimentally and theoretically for a long time.[1] A number of experimental data have been accumulated by observing x-ray and Auger-electron transitions with multiple vacancies. Theoretically, the multiple ionization can be in general treated with the independent electron model[2] and the vacancy distribution in atomic collisions is expressed according to the binomial distribution constructed from the ionization probabilities of atomic electrons concerned.[3] It is usual to use the ionization probability per i-shell electron at zero impact parameter, $p_i(0)$, for this purpose.

There have been reported several attempts to estimate $p_i(0)$ in various theoretical models. The most frequently used methods are the binary-encounter approximation (BEA)[3] and the semi-classical approximation.[4] These models give satisfactory results for multiple vacancy distributions in the case of light ion impact.[5,6] However, the ionization probability obtained by both models is proportional to Z_1^2, where Z_1 is the projectile charge. When the projectile is a multiply-ionized heavy ion, the $p_i(0)$ value sometimes exceeds the unity and the unitarity is violated.

On the other hand, Becker *et al.*[7] developed the coupled-channel method based on the independent Fermi particle model for KL^n multiple vacancy production. According to their model, the value of $p_i(0)$ tends to saturate toward the unity with increasing Z_1. However, their calculations are complicated and it is not easy to extend their model to outer-shell ionization.

Recently, Sulik *et al.*[8] proposed the geometrical model to calculate the ionization probability at zero impact parameter for high-velocity limit. Their model is based on the classical BEA of Thomson[9] and satisfies the unitarity condition for large Z_1. The

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ionization probability obtained from this model is expressed as a function of a scaling parameter Z_1/v_1, where v_1 is the velocity of the projectile, and universal for the target atomic number Z_2. Later Sulik and Hock[10] extended the geometrical model to be valid for low- and medium-velocity region.

The geometrical model is a simple, but very useful model to calculate $p_i(0)$ for an arbitrary atomic electron and to analyze the experimental data of multiple ionization processes in ion-atom collisions. The calculated ionization probabilities are known[11] to be in agreement with the experimental results as well as more elaborate coupled-channel calculations.[7]

In the previous work,[12] we have calculated the ionization probabilities at zero impact parameter in the geometrical model using the Hartree-Fock-Roothaan (HFR) wave functions[13,14] and studied the influence of the screening effect on the ionization probability. This wave function effect is larger for smaller Z_2 and for larger principal quantum number of the atomic shell. It is the purpose of the present work to test the electronic relativistic effect on the ionization probability in the geometrical model. The ionization probabilities at zero impact parameter are calculated using the relativistic hydrogenic wave functions and the results are compared with the nonrelativistic values.

2. THEORETICAL

According to the geometrical model,[8,10] the ionization probability at zero impact parameter per electron is given by

$$p_{n\kappa}(x)=1-\frac{1}{a_n^3}\int_x^\infty \mathrm{d}t\ t\ R_{n\kappa}^2(t)(t^2-x^2)^{1/2}, \tag{1}$$

where n is the principal quantum number, κ is the relativistic quantum number, x is the universal parameter, a_n is twice of the reciprocal of the Bohr radius of the electron with n and Z_2, $t=a_n r$, r is the radial distance, and $R_{n\kappa}(r)$ is the radial part of the electron wave function for $n\kappa$ shell. The quantum number κ is written as $\kappa=\mp(j+1/2)$ for $j=l\pm1/2$, where l is the orbital angular momentum and j is the total angular momentum. The parameter x is defined as

$$x=4\frac{Z_1}{v_1}V\ [G(V)]^{1/2}, \tag{2}$$

where $V=v_1/v_2$ is the scaled projectile velocity, v_2 is the velocity of the target electron, and $G(V)$ is the BEA scaling function.[3]

For the nonrelativistic hydrogenic wave function, the integral in Eq.(1) can be expressed in terms of the integral[12]

$$J_m(\mu,x)=\int_x^\infty \mathrm{d}t\ t^m e^{-\mu t}(t^2-x^2)^{1/2}, \tag{3}$$

and the final form is written analytically as a function of x by the use of the modified Bessel function of 2nd kind. In the relativistic case, the hydrogenic wave function is given by[15]

$$\psi_{n\kappa}(\mathbf{r})=\begin{pmatrix} g_{n\kappa}(r)\chi_{\kappa}^{\mu}(\hat{\mathbf{r}}) \\ \mathrm{i}f_{n\kappa}(r)\chi_{-\kappa}^{\mu}(\hat{\mathbf{r}}) \end{pmatrix}, \tag{4}$$

where $g_{nk}(r)$ and $f_{nk}(r)$ are the large and small components of the radial wave function, respectively, $\chi_{\kappa}^{\mu}(\hat{\mathbf{r}})$ is the spin-angular function, and $\hat{\mathbf{r}}$ is the unit vector of the direction of the position vector $\mathbf{r}$.

The radial wave function of the atomic number Z is expressed as

$$f_{n\kappa}(r)=-N(1-W)^{1/2}r^{\gamma-1}\mathrm{e}^{-\lambda r}\left[n\kappa F_1-\left(\kappa-\frac{Z}{\lambda}\right)F_2\right], \tag{5}$$

$$g_{n\kappa}(r)=N(1+W)^{1/2}r^{\gamma-1}\mathrm{e}^{-\lambda r}\left[-n\kappa F_1-\left(\kappa-\frac{Z}{\lambda}\right)F_2\right], \tag{6}$$

where

$$n'=n-|\kappa|,$$

$$\gamma=[\kappa^2-(\alpha Z)^2]^{1/2},$$

$$W=\left[1+\left(\frac{\alpha Z}{n'+\gamma}\right)^2\right]^{-1/2},$$

$$\lambda=Z[n^2-2n'(|\kappa|-\gamma)]^{-1/2},$$

$$F_1=F(-n'+1,\ 2\gamma+1,\ 2\lambda r),$$

$$F_2=F(-n',\ 2\gamma+1,\ 2\lambda r).$$

Here α is the fine structure constant and $F(a,b,z)$ is the confluent hypergeometric function.

From Eqs.(5) and (6), we obtain

$$R_{n\kappa}^2(r)=f_{n\kappa}^2(r)+g_{n\kappa}^2(r). \tag{7}$$

Inserting Eq. (7) into Eq. (1) and changing the variable from r to t, the ionization probability $p_{n\kappa}(x)$ can be evaluated using the numerical integration technique. In this case, the relativistic expression for a_n and x should be used. From the definition of a_n and x, these parameters for the relativistic hydrogenic wave functions can be given by

$$a_n=2\lambda, \tag{8}$$

and

$$x=\frac{2Z_1}{v_1}V[G(V)]^{1/2}\lambda\alpha\left[\frac{2}{1-W}\right]^{1/2}, \tag{9}$$

$$\approx\frac{n-(|\kappa|-\gamma)}{[n^2-2n'(|\kappa|-\gamma)]^{1/2}}\frac{4Z_1}{v_1}V[G(V)]^{1/2}. \tag{10}$$

3. RESULTS AND DISCUSSION

The ionization probabilities at zero impact parameter in the geometrical model have been calculated with the relativistic hydrogenic wave functions as a function of the parameter x. The obtained results are shown graphically in Figs. 1—14 and compared with the nonrelativistic ones. In the relativistic case, the ionization probability is not universal for Z_2. The calculations were made for copper, silver and gold from K shell to O_2 shell. In a real atom, there is no electron above N_2 shell for copper and in $N_{6,7}$ and O_2 shells for silver. However, comparison between the relativistic and nonrelativistic values is made also for the *excited* states of these atoms because it is the

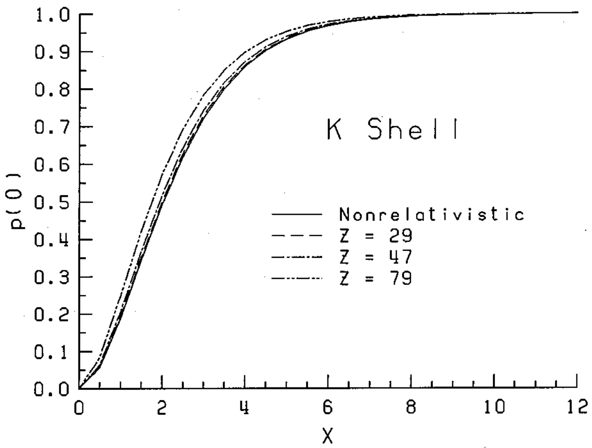

Fig. 1. The ionization probabilities per electron for K shell at zero impact parameter as a function of the parameter x. The solid curve represents the result with the nonrelativistic hydrogenic wave function, the dashed curve with the relativistic hydrogenic wave function for copper, the dot-dashed curve for silver, and the double-dot-dashed curve for gold.

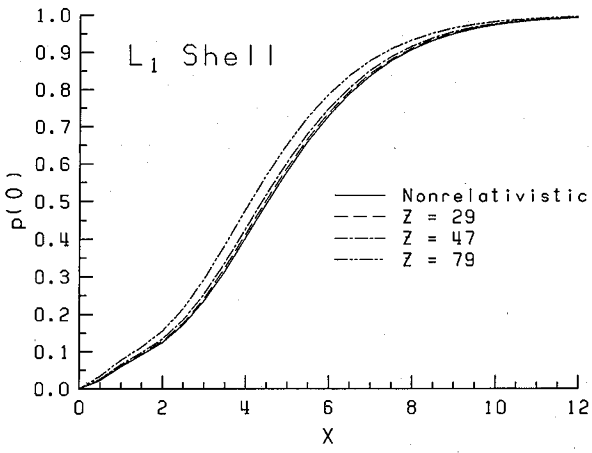

Fig. 2. The same as Fig. 1, but for L_1 shell.

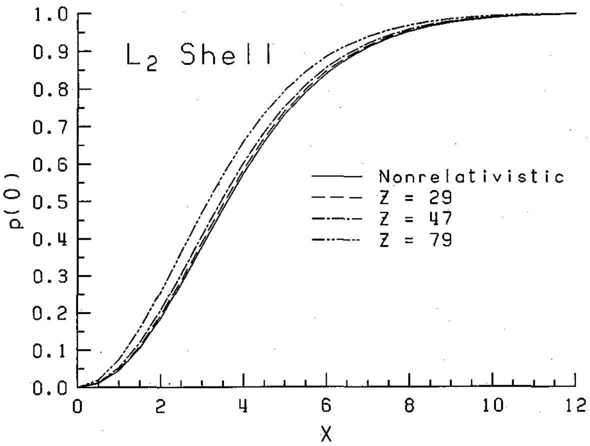

Fig. 3. The same as Fig. 1, but for L_2 shell.

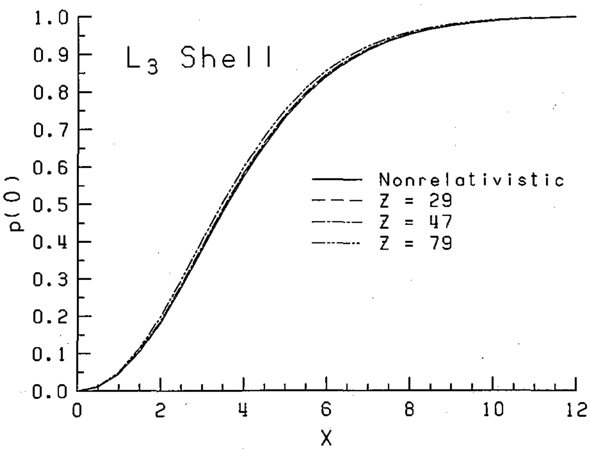

Fig. 4. The same as Fig. 1, but for L_3 shell.

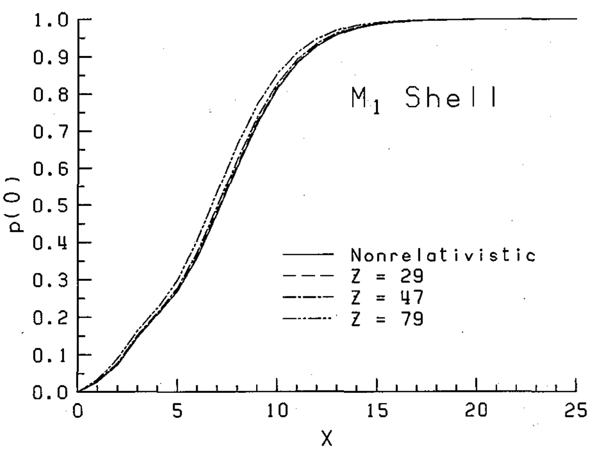

Fig. 5. The same as Fig. 1, but for M_1 shell.

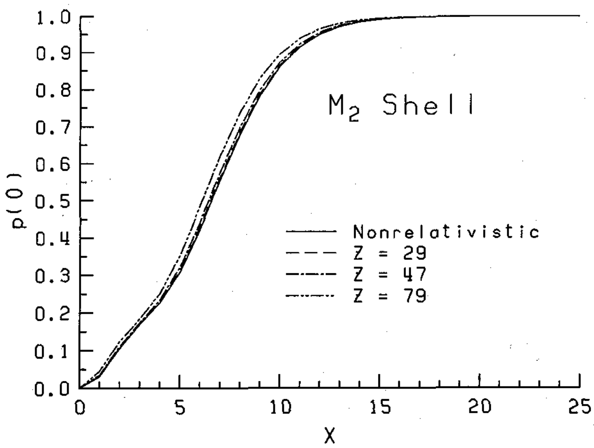

Fig. 6. The same as Fig. 1, but for M_2 shell.

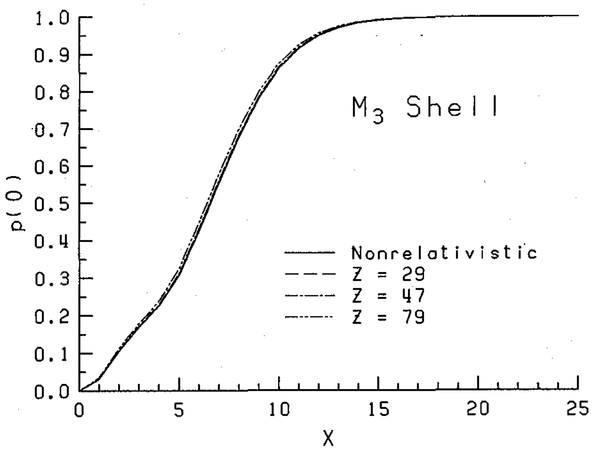

Fig. 7. The same as Fig. 1, but for M_3 shell.

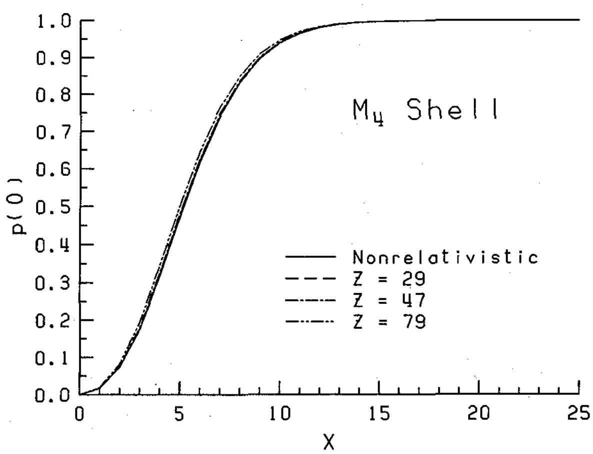

Fig. 8. The same as Fig. 1, but for M_4 shell.

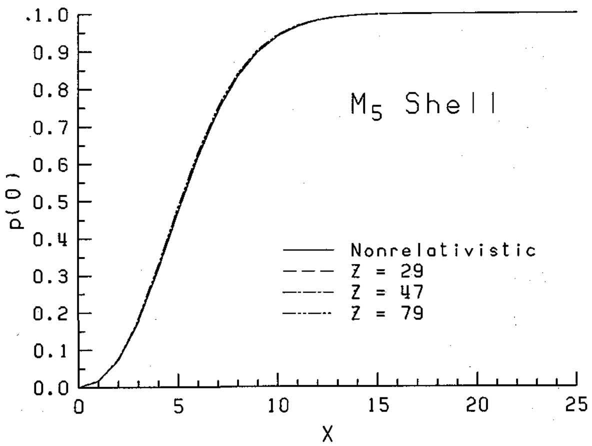

Fig. 9. The same as Fig. 1, but for M_5 shell.

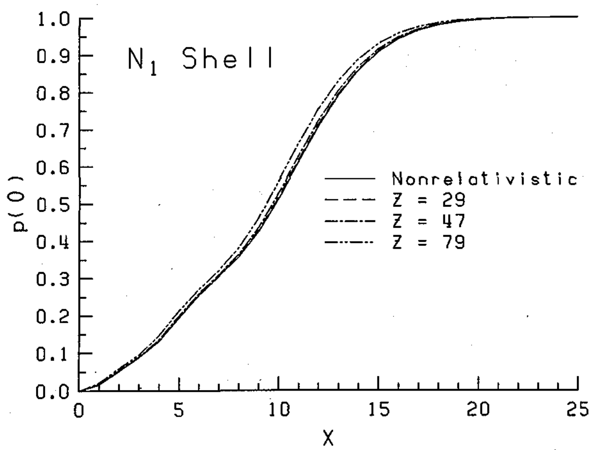

Fig. 10. The same as Fig. 1, but for N_1 shell.

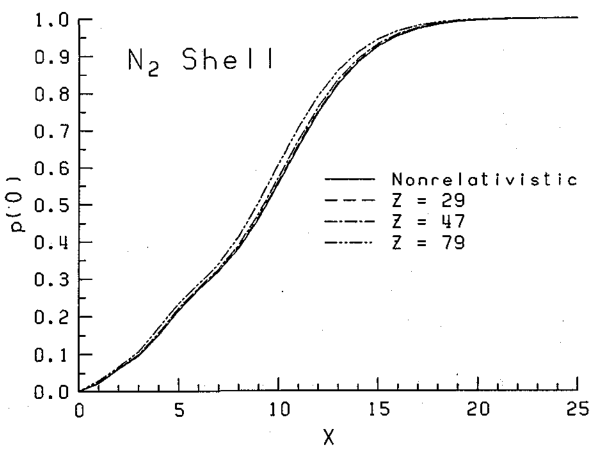

Fig. 11. The same as Fig. 1, but for N_2 shell.

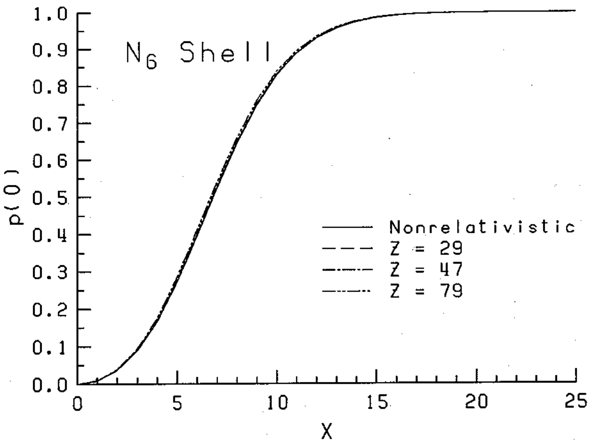

Fig. 12. The same as Fig. 1, but for N_6 shell.

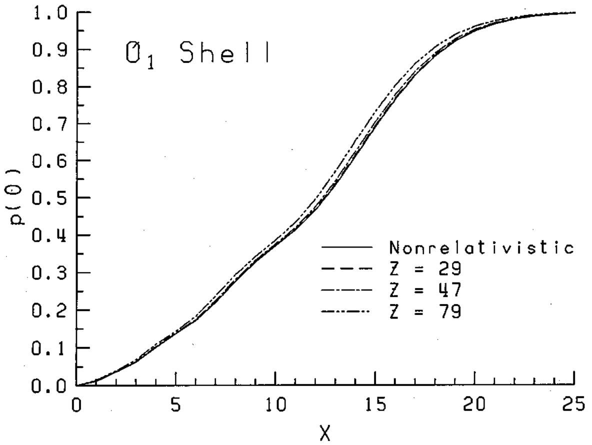

Fig. 13. The same as Fig. 1, but for O_1 shell.

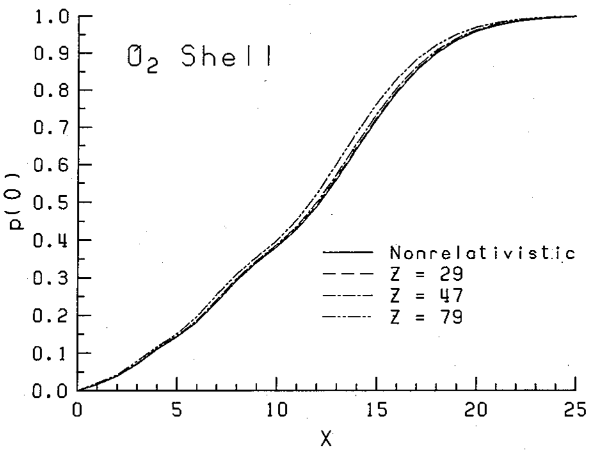

Fig. 14. The same as Fig. 1, but for O_2 shell.

main purpose of the present work to estimate the relativistic effect on the ionization probability as a function of x and Z_2.

It is clear from the figures that the relativistic effect increases the ionization probability. The increase in the probability is larger for larger Z_2 values. This fact can be explained as follows. Since the ionization probability in the present work corresponds to that with zero impact parameter with respect to the target nucleus, it is roughly proportional to the electron density at the nucleus. For the relativistic wave functions, it is well known that there is a shrink in the wave function near the nucleus. This *relativistic contraction* is the reason for the increase in the electron density at the nucleus.

The relativistic effect is large for s and $p_{1/2}$ electrons, because they have large density at the nucleus and the relativistic contraction is large. The effect is larger for inner shells by the same reason. On the other hand, the charge density of $p_{3/2}$, d and f electrons at the nucleus is small and the relativistic effect on the ionization probability for these electrons is of minor importance.

In Figs. 15—26, the relative ratios of the relativistic value to the nonrelativistic one are plotted against x. The relativistic enhancement of the ionization probability is large for small x values and decreases gradually with increasing x. This trend can be ascribed to the saturation effect of the ionization probability as a function of x.

It is interesting to note that the relativistic enhancement for $p_{1/2}$ electrons is larger than that for s electrons, while s electrons have larger density at the nucleus than $p_{1/2}$ electrons. Comparison between the relativistic and nonrelativistic wave functions indicates that the shape of nonrelativistic wave functions for l is similar to that of relativistic wave functions for $j=l+1/2$, but different from that for $j=l-1/2$. The difference in the behavior of nonrelativistic p wave functions from that of relativistic $p_{1/2}$ wave functions is large near to the nucleus and gives rise large relativistic effect for $p_{1/2}$ electrons.

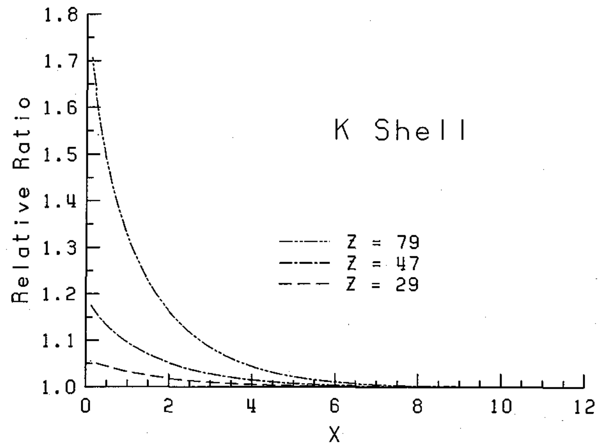

Fig. 15. Relative ratio of the relativistic ionization probability for K shell to the nonrelativistic one. The dashed curve with the relativistic hydrogenic wave function for copper, the dot-dashed curve for silver, and the double-dot-dashed curve for gold.

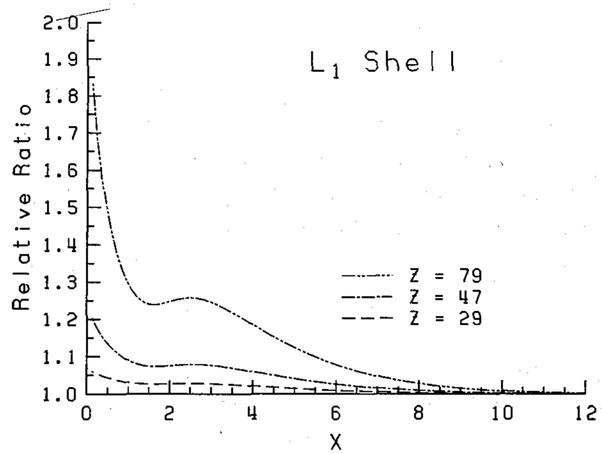

Fig. 16. The same as Fig. 15, but for L_1 shell.

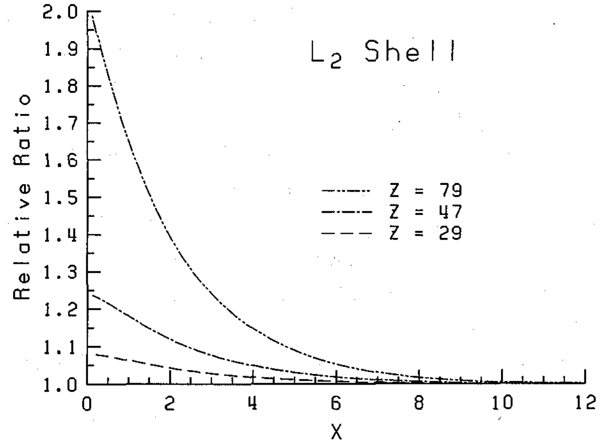

Fig. 17. The same as Fig. 15, but for L_2 shell.

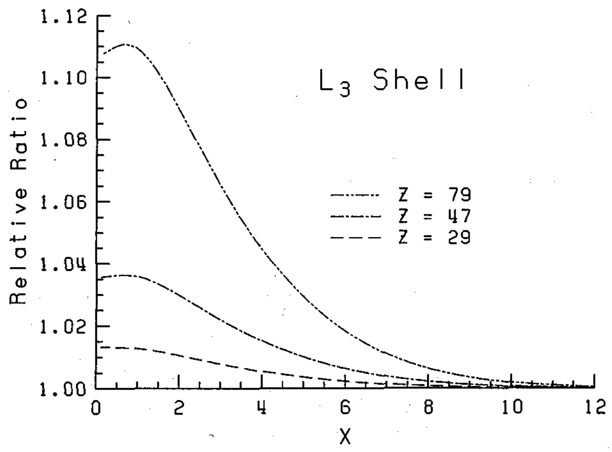

Fig. 18. The same as Fig. 15, but for L_3 shell.

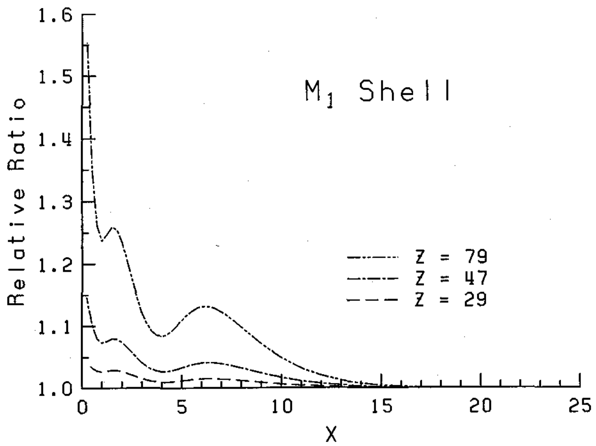

Fig. 19. The same as Fig. 15, but for M_1 shell.

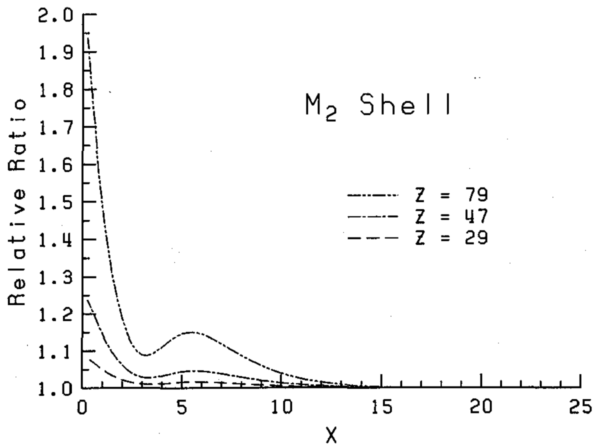

Fig. 20. The same as Fig. 15, but for M_2 shell.

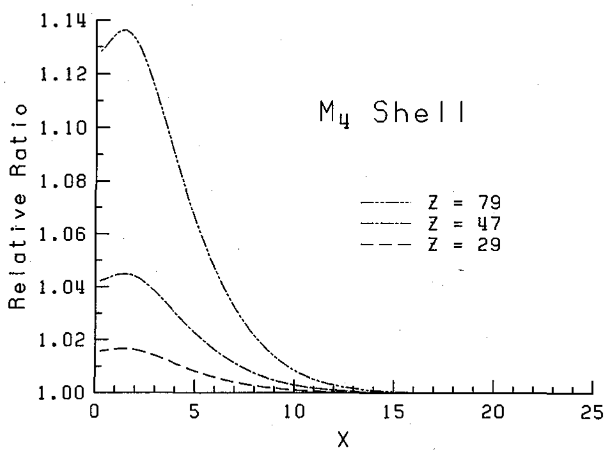

Fig. 21. The same as Fig. 15, but for M_4 shell.

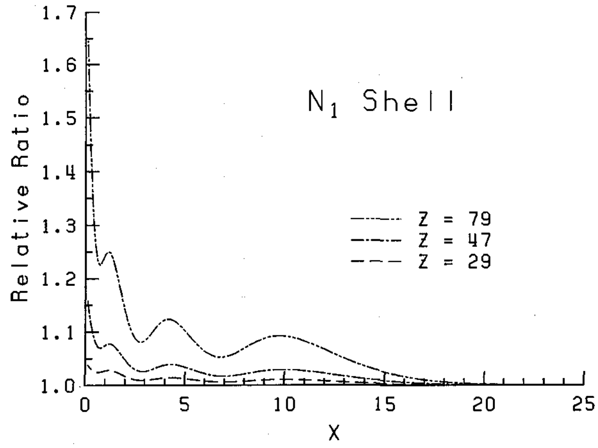

Fig. 22. The same as Fig. 15, but for N_1 shell.

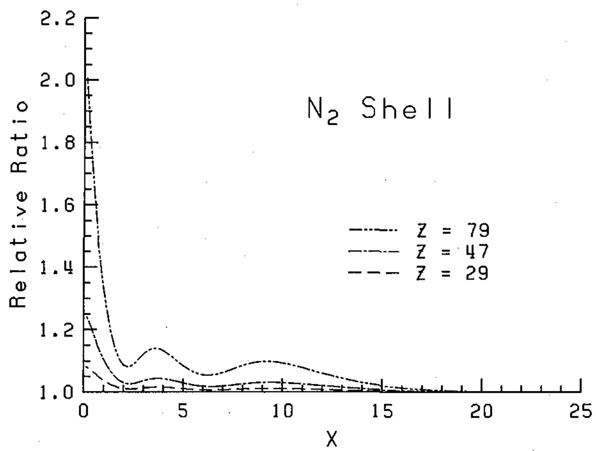

Fig. 23. The same as Fig. 15, but for N_2 shell.

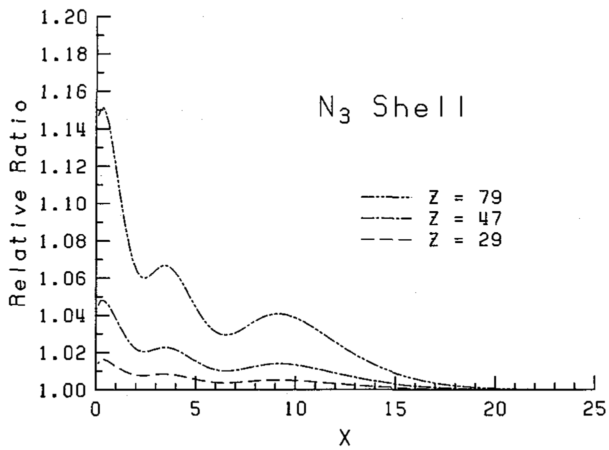

Fig. 24. The same as Fig. 15, but for N_3 shell.

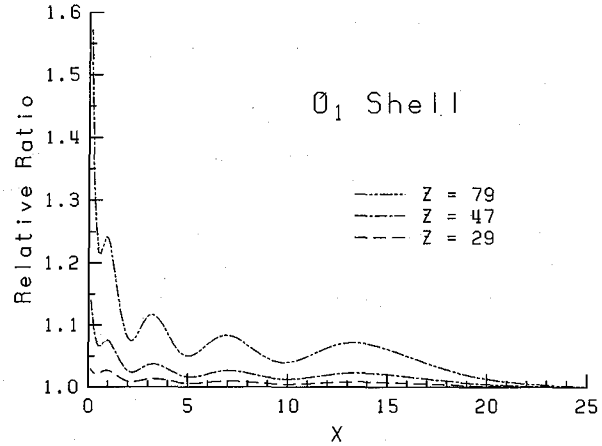

Fig. 25. The same as Fig. 15, but for O_1 shell.

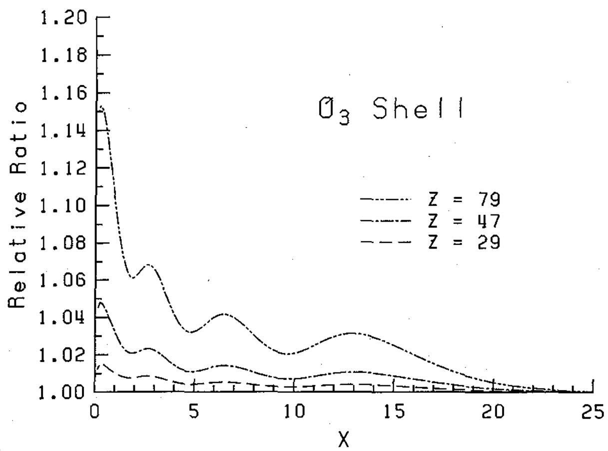

Fig. 26. The same as Fig. 15, but for O_3 shell.

When the wave function has nodes, such as in L_1, M_1, M_2 shells, the relative ratio has a structure, *i.e.* there are bumps. This structure comes from the shift in positions of nodes of the relativistic wave functions with respect to the nonrelativistic ones. As can be seen from the figures, the number of bumps corresponds to the number of nodes of the wave function.

It should be noted that the nonrelativistic hydrogenic ionization probability in the geometrical model is universal for Z_2. This fact means that the ionization probability for the screened hydrogenic model with an effective nuclear charge $Z_{eff}=Z_2-\sigma$ defined by a screening constant σ is same as that for the hydrogenic model, though the value of x in Eq. (2) changes. On the other hand, in the relativistic case the screened hydrogenic model yields the ionization probability different from the hydrogenic model. In the present work, we used the relativistic hydrogenic wave function and estimated the relativistic effect as a ratio to the nonrelativistic hydrogenic (or screened hydrogenic) result. If we introduce an appropriate screening constant $\sigma\geqq 0$ and use the effective nuclear charge in the relativistic hydrogenic wave function, the relativistic effect decreases. However, the ionization probability depends on σ and there arises a new problem how to choose σ.

In conclusion, we have calculated ionization probabilities at zero impact parameter with relativistic hydrogenic wave functions and shown that the relativistic effect increases the ionization probability. The enhancement is larger for small x values, for heavy elements, and for inner-shell s and $p_{1/2}$ electrons. In our previous work,[12] we have already shown that the wave function effect is larger for smaller Z_2 elements and for outer-shell electrons. Considering both results, we can say in general that the relativistic effect is important for large Z_2 elements and the wave function effect plays an important role for small Z_2 atoms. Therefore, in order to obtain more realistic ionization probabilities for small x values, both relativistic and wave function effects should be taken into consideration simultaneously. Such calculations are being in progress.

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